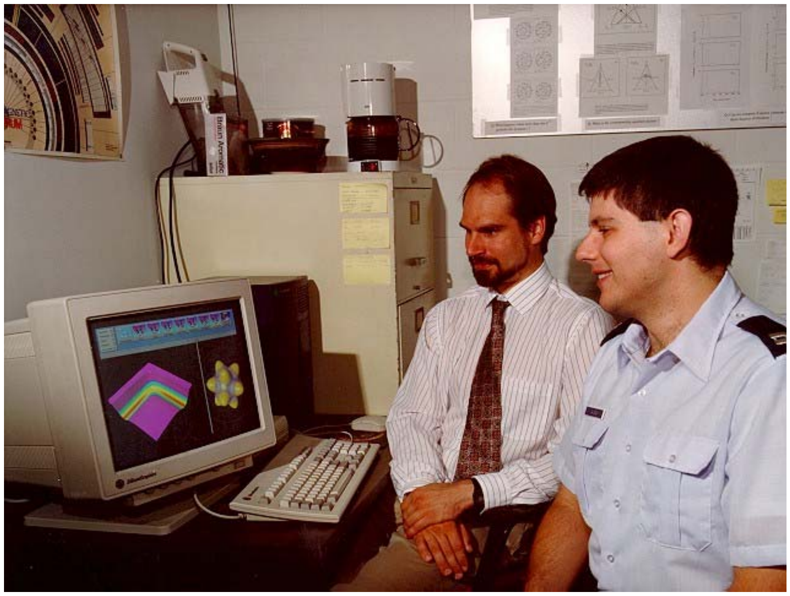

COMPUTATIONAL PHYSICS

The Department of Engineering Physics is actively pursuing research in the Department of Defense critical technology areas of computational fluid dynamics, computational electronics and nano-electronics, and computational chemistry and materials science. The computational resources of AFIT are significantly enhanced by the presence of one of the four Major Shared Resource Centers of the Department of Defense at Wright Patterson. Currently five faculty members and eight graduate students are pursuing research in the computational physics area.

Theoretical work in computational fluid dynamics involves the study of non-equilibrium kinetics and chemistry of both high density and low density plasmas. This research activity includes: modeling of the magnetosphere and ionosphere, shock structure in ionizing flows, and the application of non-local kinetics to plasma processing of materials. Computer simulation of plasma phenomena is an established yet rapidly changing practice. Our research in this area is based on a theoretical description of plasmas with viewpoints ranging from the microscopic to the macroscopic. A microscopic approach is adopted in the development of solutions of the collisional Boltzmann equation. We are currently exploring the use of an adaptive energy mesh to increase the accuracy and computational efficiency of such calculations, as well as solutions appropriate to the non-local conditions found in plasma processing reactors and thermionic converters. Particle simulations, based on particle-in-cell models coupled with Monte Carlo techniques, complement the Boltzmann approach and permit alternative investigations of non-local phenomena. These studies are directed toward the characterization of RF and inductive discharges and Langmuir probe diagnostics in hypersonic flows. A macroscopic approach, based on moments of the Boltzmann equation, is also employed in magneto-hydrodynamic studies of space plasmas, collision dominated plasmas, shock modification in ionized flows, and the forecasting of magnetospheric disturbances and their influence on space assets. These studies contribute to the modeling and validation of operational AF codes characterizing the space environment, as well as characterizing high-latitude GPS scintillation and ionospheric plasma dynamics.

Studies in the critical technology areas of nanoelectronics and materials science have a quantum mechanical focus. Research interests in this area range from computational and theoretical chemistry, involving rovibrational dynamics and spectroscopy of polyatomic molecules, rotation-vibration coupling and non-linear dynamics to solid-state physics, addressing quantum well structures and applied group theory. We developing and applying quantum computational methods to model surface and bulk chemical properties. Particularly of interest is to model the interfaces and defects in semiconducting materials with increasing size scale from molecules to solid state. Currently applications are being made to silicon, silicon carbide and uranium oxides.

FACULTY:

Bailey, William F.
Associate Professor of Physics
B.S., United States Military Academy, 1964; M.S., The Ohio State University, 1966; Ph.D., AF Institute of Technology, 1978. Transport properties in weakly ionized and reactive gas mixtures with applications to space environmental modeling, gas discharges, and thermionic energy conversion.

Burggraf, Larry W.
Associate Professor of Engineering Physics, Dept of Engineering Physics.
B.A., Olivet Nazarene University, 1968; M.S., Ohio State University, 1971; M.A., University of West Florida, 1977; Ph.D., University of Denver, 1981: detection of trace chemicals and radionuclides by optical and nuclear techniques using selective preconcentration; quantum calculations to model adsorbate interactions with surfaces, especially silica and alumina; and optical spectroscopy of nuclear fuels.

Garscadden, Alan
Adjunct Professor
B.S., Queens University, Belfast, 1958; Ph.D., Queens University, Belfast, 1962. Physics of low-energy plasmas with an emphasis on kinetics far from equilibrium in flames, discharges, and arcs. Spectroscopic diagnostics of plasmas and flames including coherent anti-Stokes Raman scattering, optogalvanic spectroscopy, and cluster formation in plasmas and flames.

Mathews, Kirk A.
Associate Professor of Nuclear Engineering.
B.S., California Institute of Technology, 1971; M.S., AFIT, 1982; Ph.D., AFIT 1983. Neutral particle (neutron, gamma-ray, x-ray) radiation transport computational methods; weapons effects simulation; radiation spectrum unfolding.

Weeks, David E.
Assistant Professor of Physics
B. A. , Colgate University, 1983; M. S. , Georgia Institute of Technology, 1985; Ph.D. , University of Arkansas, 1989. Modeling of magnetosphere, computer simulations, molecular reaction dynamics.

SOME RECENT PUBLICATIONS:

“Photoelectron spectroscopy of $Si_2C_3^-$ and quantum chemistry of the linear Si_2C_3 cluster and its isomers”, X. Duan, L.W. Burggraf, D.E. Weeks, C. Lineberger et al., J. Chem. Phys., Vol. 116, no. 9, 3601-3612, 2002.

“The Physics of Vibration-Dissociation Coupling in Hpersonic Flows,” 32nd AIAA Plasmadynamics and Lasers Conference, 11-14 June 2001, Anaheim, CA, E. Josyula and Wm. F. Bailey.

“Vibration-Dissociation Coupling Using Master Equations in Nonequilibrium Hypersonic Blunt Body Flow,” 31st AIAA Plasma Dynamics and Lasers Conference 19-22 June 2000, Denver CO, E. Josyula and Wm. F. Bailey.

“An Ab Initio Cluster Study of the Structure of the Si(001) Surface”, J.R. Shoemaker, L.W. Burggraf and M.S. Gordon, Journal of Chemical Physics, Vol. 112, No. 6, 2994-3005, 2000.

"Vibration-Dissociation Coupling Using Master Equations in Nonequilibrium Hypersonic Blunt Body Flow," Journal of Thermophysics and Heat Transfer, Vol. 15, Number 2, 157-167, (April-June 2001).

“Scattering Matrix Elements and Cross Sections for the Reaction B (2P1/2) + H2 (j) <-> B (2P3/2) + H2 (j Œ),² Proceedings of the High Energy Density Matter (HEDM) Contractors,” Conference Held 24-26 October 2000 in Park City UT, AFOSR Technical Report, D.E. Weeks, S.H. Yang, and T.A. Niday.

“Scattering Matrix Elements for the Fine Structure Transition, B (2P1/2) + H2 (j = 0) <-> B (2P3/2) + H2 (j = 0),” Chem. Phys. Letters 308 (1999) 106-114, T.A. Niday and D.E. Weeks.

“Scattering Matrix Elements for the Fine Structure Transition B (2P1/2) + H2 (j = 0) <-> B (2P3/2) + H2 (j = 0),” Proceedings of the High Energy Density Matter (HEDM) Contractors’ Conference Held 8-10 June 1999 in Cocoa Beach FL, AFOSR Technical Report, T. A. Niday and D. E. Weeks.

“A New Application of the Interaction Picture to Calculate Reactive Scattering Matrix Elements,” J. Phys. Chem. A 102 (1998) 9489-9493, M.J. MacLachlan and D.E. Weeks.

“Time Dependent Wave-packet Studies of the Reaction HO + CO <-> H + CO2,” Proceedings of the High Energy Density Matter (HEDM) Contractors’ Conference Held 20-22 May 1998 in Monterey CA, AFOSR Technical Report, D.E. Weeks and R.S. Calfas.

“An Application of the Interaction Picture to Calculate S-Matrix Elements for Reactive Scattering,” Proceedings of the High Energy Density Matter (HEDM) Contractors’ Conference Held 1-3 June 1997 in Chantilly VA, PL - TR - 97 - 3057, March 1998, M.J. MacLachlan and D.E. Weeks.

“Comparison of Measured and Computed Strehl Ratios for Light Propagation Through a Channel Flow of a $He\text{-}N_2$ Mixing Layer at High Reynolds Numbers,” P. J. Gardner, M. C. Roggemann, B. M. Welsh, R. D. Bowersox, and T. E. Luke, Applied Optics, vol 36, pp 2559-2567; April 1997.

“A New Application of Absorbing Boundary Conditions for Computing Collinear Quantum Reactive Scattering Matrix Elements,” Chem. Phys. Letters 263 (1996) 292-296, R.S. Calfas and D.E. Weeks.

"Measurements of O_3, H_2O and ClO in the Middle Atmosphere using the Millimeter-wave Atmospheric Sounder (MAS)”, Geophysical Research Letters, Vol. 23, No. 17, 1996, Goldizen et al.

"Determination of the Self-Consistent Space Charge Potential Using the Non-local Approach”, Eric J. Bennett and Wm. F. Bailey, Bulletin of the American Physical Society, Vol 41, No 6, October 1996, 1344.

“Upcoming Ionospheric Impacts on GPS at Solar Max-- What do we know/What do we need?” Proceedings of ION (Institute of Navigation) GPS-96, Kansas City, MO, 1996, Goldizen et al.

“An Integrated Molecular Orbital/Molecular Mechanics Optimization Scheme For Surfaces, SIMOMM”, J.R. Shoemaker, L.W. Burggraf and M.S. Gordon, J. Phys. Chem. A, 103, 3245 (1999).